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**1997 GORDON RESEARCH CONFERENCE
on GASEOUS IONS, STRUCTURE, ENERG. & REACT.
FINAL PROGRESS REPORT**

**AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
GRANT NO. F49620-97-1-0065**

The Gordon Research Conference (GRC) on GASEOUS IONS, STRUCTURE, ENERG. & REACT. was held in Ventura, California at DOUBLETREE HOTEL from 2/23/97 thru 2/28/97. The Conference was well-attended with 130 participants (attendees list attached). The attendees represented the spectrum of endeavor in this field coming from academic, industry, and government laboratories, both U.S. and foreign scientists, senior researchers, young investigators, and students.

In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field. There was a conscious effort to stimulate lively discussion about the key issues in the field today. Time for formal presentations was limited in the interest of group discussions. In order that more scientists could communicate their most recent results, poster presentation time was scheduled. Attached is a copy of the formal schedule and speaker program and the poster program. In addition to these formal interactions, "free time" was scheduled to allow informal discussions. Such discussions are fostering new collaborations and joint efforts in the field.

I want to personally thank you for your support of this Conference. As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings. If you wish any further details, please feel free to contact me. Thank you.

Sincerely,


ROBERT SQUIRES
PURDUE UNIVERSITY

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Gordon Research Conference

Structures, Energetics and Dynamics of Gaseous Ions

**February 23 - 27, 1997
Doubletree Hotel, Ventura California**

R. R. Squires, Chair T. Baer, Vice Chair

Program

Sunday, February 23

- 2:00 PM Registration
4:30 - 6:00 Reception & Poster Session I
6:00 - 7:00 Dinner
7:00 - 7:15 Opening Remarks/Announcements

Evening Session: Ion-Surface Interactions

- 7:15 - 7:30 Discussion Leader: Steve Bernasek, Princeton University
7:30 - 8:30 Graham Cooks, Purdue University
Dissociation, Reactions and Soft-Landing of Ions at Surfaces
8:30 - 9:30 Vicki Wysocki, University of Arizona
Two Different Facets of Ion-Surface Collisions: Peptide Dissociation and Dependence of Reactions on Orientation of Surface Chains
9:30 - 10:30 Poster Session I, con'd

Monday, February 24

7:30 - 8:30 Breakfast

Morning Session: Organic Mechanisms

8:45 - 9:00 Discussion Leader: Helmut Schwarz, Technical University of Berlin

9:00 - 10:00 Chuck DePuy, University of Colorado at Boulder
Gas-Phase Electrophilic Substitution: CH₃⁺ vs. BH₂⁺

10:00 - 10:20 Break

10:20 - 11:20 John Holmes, University of Ottawa-Carleton
Ion Structure Assignment; Certainty and Speculation

11:20 - 12:20 Hans Grützmacher, University of Bielefeld
Some Aspects of the Bimolecular Reactivity of Unsaturated Organic Radical Cations

12:30 - 1:30 Lunch

4:30 - 6:00 Poster Session II

6:00 - 7:00 Dinner

Evening Session: Atmospheric Chemistry/New Faces

7:15 - 7:30 Discussion Leader: Carl Howard, NOAA

7:30 - 8:30 Greg Huey, NOAA
Ion Chemistry for the Selective Detection of HNO₃ and Other Important Atmospheric Species

8:30 - 9:30 Kim Prather, University of California at Riverside
Real-Time Analysis of Atmospheric Aerosols

9:30 - 10:30 Poster Session II, con'd

Tuesday, February 25

7:30 - 8:30 Breakfast

Morning Session: Reaction Dynamics

8:45 - 9:00 Discussion Leader: Doug Ridge, University of Delaware

9:00 - 10:00 Chava Lifshitz, The Hebrew University of Jerusalem
Time-Resolved Studies of PAHs and Fullerenes

10:00 - 10:20 Break

10:20 - 11:20 Rob Dunbar, Case Western Reserve University
Binding Metal Ions to Planar π -Systems

11:20 - 12:20 Seung-Koo Shin, University of California at Santa Barbara
Time- and Product-Resolved Photodissociation of Toluene and Halotoluene Radical Cations

12:30 - 1:30 Lunch

4:30 - 6:00 Poster Session III

6:00 - 7:00 Dinner

Evening Session: Theory

7:15 - 7:30 Discussion Leader: Scott Gronert, San Francisco State University

7:30 - 8:30 Bill Hase, Wayne State University
Trajectory Studies of Energy Transfer in the Reaction and Dissociation of Gaseous Ions

8:30 - 9:30 Wes Borden, University of Washington
Gas-Phase Ion Chemistry as a Tool for Investigating Organic Molecules of Theoretical Interest -- The Synergy between Calculations and Experiments

9:30 - 10:30 Poster Session III, con'd

Wednesday, February 26

7:30 - 8:30 Breakfast

Morning Session: Biological/Electrospray Ionization

8:45 - 9:00 Discussion Leader: Julie Leary, University of California at Berkeley

9:00 - 10:00 Scott McLuckey, Oak Ridge National Laboratory
Gas-Phase Bio-Ion/Ion Chemistry in the Paul Trap

10:00 - 10:20 Break

10:20 - 11:20 Evan Williams, University of California at Berkeley
Blackbody Infrared Radiative Dissociation of Large Biomolecule Ions: A Route to Energetics and Dynamics

11:20 - 12:20 Mike Bowers, University of California at Santa Barbara
Conformations of Biologically Interesting Molecules in the Gas Phase: The Latest News

12:30 - 1:30 Lunch

1:30 - 2:00 Business Meeting to Select New Vice-Chair

4:30 - 6:00 Poster Session IV

6:00 - 7:00 Dinner

Evening Session: Molecular Clusters

7:15 - 7:30 Discussion Leader: Will Castleman, Pennsylvania State University

7:30 - 8:30 Michael Mautner, NIST & University of New Zealand
Multi-body Cooperative Processes: New Reactions Observed in Ionic Polymerization

8:30 - 9:30 Al Viggiano, Phillips Laboratory
Thermal Energy Reactions of Cluster Ions

9:30 - 10:30 Poster Session IV, con'd

Thursday, February 27

7:30 - 8:30 Breakfast

Morning Session: Spectroscopy/Threshold Ionization

8:45 - 9:00 Discussion Leader: Mark Johnson, Yale University

9:00 - 10:00 Carl Lineberger, JILA/University of Colorado at Boulder
Time-Resolved Dynamics in Large Cluster Ions

10:00 - 10:20 Break

10:20 - 11:20 Ed Grant, Purdue University
State-to-State Dynamics of Polyatomic Photoionization

11:20 - 12:20 Klaus Müller-Dethlefs, University of York
Structure and Dynamics of Molecular Ions and Clusters Studied by ZEKE Spectroscopy

12:30: - 1:30 Lunch

6:00 - 7:30 Conference Banquet

Evening Session: Featured Speaker

7:30 - 7:40 Introduction: Bob Squires

7:40 - 8:40 Eldon Ferguson, NOAA
Flowing Afterglow Studies of Ion-Molecule Reactions, 1964-1996

9:00 - 12:00 Social with Live Music

Friday, February 28

departure

1997 Gaseous Ions Gordon Conference Poster Sessions

Sunday Posters

1. Size Selective Protonation within $(ROH)_n(H_2O)H^+$ Cluster Ions

Michael M. Y. Lyktev, Robert L. DeLeon, and James F. Garvey

Department of Chemistry, Natural Sciences & Mathematics Complex

State University of New York, University at Buffalo, Buffalo, NY 14260-3000

2. Metal-ion chemistry in Clusters Initiated by Ionization/Dissociation of Organometallic Precursors

S. Bililign[‡], L. Liu, C. S. Feigerle and John C. Miller

Chemical and Biological Physics Section, Oak Ridge National Lab, PO Box 20008; Oak Ridge, TN 831 and

Department of Chemistry, University of Tennessee, Knoxville, TN 996

[‡] Also at Physics Department, North Carolina A&T State University, 1601 East Market St., Greensboro, NC 27411.

3. On the Dynamical Shell Structure of Hydrogen Cluster Ions

S. Schlemmer, W. Paul, and D. Gerlich

Technical University Chemnitz, Germany

4. H^+ , Li^+ , and Na^+ Affinity Study of N_2 , P_2 and their Isoelectronic Species

Yu-Nung Su, Ming-Sung Tsai, and San-Yan Chu

Department of Chemistry, National Tsing Hua University, Taiwan

5. The Gas-phase Complex [$t-C_4H_9^+/1,4\text{-Benzylbicyclo[2.2.2]octane}$]

Dietmar Kuck, Carsten Matthias and Björn Bredenkötter

Department of Chemistry, University of Bielefeld, Germany

6. Treatment of Competitive Dissociation Processes by Threshold Collision-Induced Dissociation.

Implications for the Kinetic Method.

P. B. Armentrout, and Mary T. Rodgers

Department of Chemistry, 3516 Henry Eyring Building, University of Utah, Salt Lake City, UT 84112

7. Formation and Rearrangements of Ion-Molecule Complexes Between Ethylene and Acetylene

Thomas Bally¹, G. Narahari Sastry¹, Petr Carsky², Pavel Jungwirth², Vojtech Hrouda², and Martina

Roeseloya²

1) Institut de Chimie Physique, Universite de Fribourg, CH-1700 Fribourg, Switzerland

2) Academy of Sciences of the Czech Republic, Prague

8. Rate Constants for the Reactions of O^+ with N_2 and O_2 and N^+ and N_2^+ with O_2 as a Function of Temperature (300-1800K).

I. Dotan,^a P.M. Hierl,^b J.V. Seeley, J.M. VanDoren,^c R.A. Morris and A.A. Viggiano

Phillips Laboratory, Geophysics Directorate, Ionospheric Effects Division (GPID); 29 Randolph Rd.

Hanscom AFB, MA 01731. a) The Open University of Israel, 16 Klausner St., Ramat-Aviv, Tel-Aviv, ISRAEL. b) Department of Chemistry, University of Kansas, Lawrence, KS 66045. c) Department of Chemistry, College of the Holy Cross, Worcester, MA 01610.

9. Spectroscopy of Transition Metal Ions and Coordination Complexes in Cluster Environments

Thomas G. Spence, Brett T. Trotter, and Lynmarie A. Posey

Department of Chemistry, Vanderbilt University, Station B. Box 1822, Nashville, TN 37235

10. Carbanion Chemistry: Recent Results

Steven Kass, Michael Hare, Dana Reed, Kathy Broadus, and Tina Arrowood

University of Minnesota, Department of Chemistry, 207 Pleasant St. S.E., Minneapolis, MN 55455

11. PTR-MS: Medical applications, food research and air quality

W. Lindinger, A. Jordan, A. Hansel, C. Warneke, R. Holzinger, P. Prazeller, and W. Vogel

Institut für Ionenphysik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, AUSTRIA

12. The ground state (1A_1) and the lowest triplet state (3B_1) of the phenyl cation $C_6H_5^+$ revisited

Jan Hrušák,^{a,c} Detlef Schröder,^b and Suehiro Iwata^c

a) Academy of Sciences of the Czech Republic, J. Heyrovsky Institute of Physical Chemistry, CZ-18223

Prague 8, Czech Republic. b) Institut für Organische Chemie der Technischen Universität Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany. c) Institute for Molecular Sciences, Myodaiji, Okazaki 444, Japan

13. Rate Constants for the Reactions of Chloride Ion with Methyl Bromide and with n-Butyl Bromide over the Pressure Range, 300 to 1100 Torr, by Ion Mobility Spectrometry

W.B. Knighton , K.E. Sahlstrom, and E.P. Grimsrud

Department of Chemistry, Montana State University, Bozeman, Montana 59717

14. Surface induced dissociation (SID) of benzene ions on self-assembled monolayer surface (SAM) by FT-ICR

Wenqing Zhong, Eugene Nikolaev*, Jean Futrell, and Vicki Wysocki**

Department of Chemistry, University of Delaware, Newark, DE 19716

*Institute of energy Problems of Chemical Physics, Russian Academy of Sciences, Russia

**Department of Chemistry, University of Arizona, Tucson, AZ 85721

15. Infrared Spectra of Molecular Ions Formed from SF₄ and SF₆ and Trapped in Solid Neon

Marilyn E. Jacox, Catherine L. Lugez, Rollin A. King, and H. F. Schaefer III

Optical Technology Division, National Institute of Standards and Technology

Gaithersburg, Maryland 20899

16. H⁻ transfer in reactions of acetylene and ethylene cations with small hydrocarbons

H. Palm, C. Alcaraz, D. Berthomieu, M. Fieber-Erdmann*, Z. Herman**, and O. Dutuit

LPCR and LURE, Centre Universitaire Paris-Sud, 91405- Orsay Cedex, France

*Synchrotron Strahlung AS, Hahn-Meitner Institut, D-14109, Berlin, Germany

**J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Dolejskova 3, 182 23 Prague 8, Czech Republic)

17. The Acidities and Basicities of Doubly Charged Ions: An ab initio Study.

Scott Gronert

Department of Chemistry and Biochemistry, San Francisco State University

San Francisco, CA 94132

18. Hydrogen Bonding in the Gas Phase: Lessons from the Potential Energy Surface

Michael L. Chabinyc and John I. Brauman

Department of Chemistry, Stanford University, Stanford CA 94305-5080

19. Stereoselective β -Hydrogen Elimination from ESI-generated Nickel(II) N-Glycoside Complexes

Glenn Smith, Steven F. Pedersen, and Julie A. Leary

Department of Chemistry, University of California, Berkeley, CA 94720

20. Gaseous Ionized Alkylphosphines: a Rich Source of Distonic Phosphorus-Containing Ions

Helmut Keck, Andreas Schweighofer

Heinrich-Heine-Universität Düsseldorf, Institut f. Anorganische Chemie und Strukturchemie

Universitätsstr. 1, D-40025 Düsseldorf, Germany

21. VUV Peaks in Absorption Spectra and in Photoion Yield Curves of Polycyclic Aromatic

Hydrocarbons and Related Compounds

S. Leach^a, H.W. Jochims^b, E.Rühl^b, H. Baumgärtel^b, and S. Tobita^{a,b}

a) Departement Atoms et Molecules en Astrophysique, URA812, Observatoire de Paris-Meudon, 92195

Meudon, France

b) Institut für Physikalische und Theoretische Chemie, der Freien Universität Berlin, Takustr. 3 14195 Berlin, Germany

22. Generation of Intense Cluster Ion Beams Through High Voltage Discharge Ionization and Ablation

Carlos Manzanares and Ansgar Brock

Department of Chemistry, Baylor University, Waco, Texas 76798

23. A SIFT Study of the Reactivity of Cations Derived from Naphthalene with Molecules and Atoms

Valery LePage, Veronica Bierbaum and Theodore P. Snow

Department of Chemistry and Biochemistry, and Center for Astrophysics and Space Astronomy, University of Colorado, Boulder CO, 80302

Monday Posters

1. Thermal Dissociation Of Acetophenone Molecular Ions Activated By Incoherent Infrared Radiation

Marcelo Sena and José M. Riveros

Instituto de Química, Universidade de São Paulo, Caixa Postal 26077, São Paulo, Brazil, CEP 05599-970

2. Strength of alkali metal coordination to N-acetylglucosamine sugars determined by on and off-resonance CID/MALDI/FTMS

Carlito B. Lebrilla, Mark T. Cancilla, Sharon G. Penn

Department of Chemistry, University of California, Davis, CA 95616

3. Theoretical Determination of Glycine Affinity for Li⁺, Na⁺, K⁺, Rb⁺, Cs⁺, Al⁺, and Cu⁺

S. Hoyau and G. Ohanessian

Laboratoire des Mecanismes Reactionnels, Department de Chimie, URA CNRS 1307
Ecole Polytechnique, 91128 Palaiseau Cedex, FRANCE

4. True Gas Phase Protein Sequencing Strategies using Mass Spectrometry: Mechanisms and Energetics of Highly Specific Cleavage Processes

Sang-Won Lee, and J. L. Beauchamp

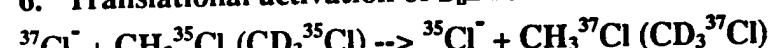
Mail Stop 127-72, California Institute Technology, Pasadena, CA 91125

5. Metal Ion Binding to Biomolecules. Attachment Sites from Bond Energies and Entropy Effects

Chrys Wesdemiotis and Blas A. Cerdá

Department of Chemistry, The University of Akron, Akron, OH 44325-3601

6. Translational activation of S_n2 reactions:



Kent M. Ervin, Vincent F. DeTuri, and Paul A. Hintz

Department of Chemistry/216, University of Nevada, Reno, NV 89557

7. Symmetric and Unsymmetric Halide-Halide interactions. Some examples of Two-Center Three-Electron Bonds.

Andreas J. Illies and Linda S. Nichols

Department of Chemistry, Auburn University, AL 36849-5314

8. State Selective Ion-Molecular Reaction: C₂H₂⁺ + NH₃

Jun Qian, Hunghsin Fu, and Scott Anderson

Department of Chemistry, University of Utah, Salt Lake City, UT 84112

9. Zero-pressure thermal radiatively induced dissociation (ZTRID) in the 'virtual' low pressure regime.

Timothy L. Hoffman and Terrance B. McMahon

Chemistry Department, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

10. SIFDT study of the formation and dissociation of CO-N₂⁺ ions in a nitrogen buffer

W. Lindinger, J. Glosik, G. Bano, and E.E. Ferguson

Institut für Ionenphysik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, AUSTRIA

11. Gas phase ion-molecule reactions as models for ion surface collision association reactions

Steven L. Bernasek, Lynn M. Phelan, Julie Flynn, Scott B. Ficarro, and Mark J. Hayward

Department of Chemistry, Princeton University, Princeton, NJ 08544

12. Reactions of methyl cations with small hydrocarbons: Hydride ion transfer and other direct mechanisms

Stefan Mark* and Dieter Gerlich

Institut für Naturwissenschaften, Technische Universität, Reichenhainer Str. 70 D-09107 Chemnitz, Germany
and a) Department of Chemistry, University of California, Berkeley, CA 94720-1460

13. Rare Gas Mediated Methane Activation by Small Transition Metal Cluster Cations
Gerhard Albert, Christian Berg, Martin Beyer, Uwe Achatz, Stefan Joos, Gereon Niedner-Schattburg, and
Vladimir E. Bondybey
Institut für Physikalische und Theoretische Chemie, TU München, Lichtenbergstrasse 4, 85356 Garching,
Germany

14. Photoelectron Spectroscopy of Ions Derived from Cyclooctatetraene
Paul G. Wenthold, and W. Carl Lineberger
JILA, Campus Box 440, University of Colorado, Boulder, CO 80309

15. Dynamics of ion molecule reactions in clusters
A.W. Castleman, Jr., E.M. Snyder, D.A. Card, D.E. Folmer, S. Sato, and S.A. Buzzo
Department of Chemistry, 152 Davey Laboratory, The Pennsylvania State University
University Park, PA 16802

16. A study of the dissociation of CH_3SH^+ by collisional activation: Observation of non-statistical behavior
P.T. Fenn, S. Stimson, and C.Y. Ng
Department of Chemistry, Iowa State University, Ames, IA 50011

17. A model calculation on interactions between alkali metals and a Si surface: an *Ab- initio* MO study
Akira Shimizu and Hiroto Tachikawa
Graduate School of Engineering, Hokkaido University, Sapporo 060, Japan

18. Intrinsic Reactivity of Metal-Hydroxide Complexes with Electrophiles: Gas-Phase Reactions of $[\text{Cp}_2\text{ZrOH}]^+$ Cations with Alcohols, Amines, Ethers, and Carboxylic Acid Derivatives.
Matthew F. Ryan, David E. Richardson, and John R. Eyler
Department of Chemistry and Physics, Purdue University Calumet, Hammond, IN 46323

19. The interstellar Haber-Bosch process
Murray J. McEwan, Graham B. Scott, David A Fairley, and Colin G. Freeman
Department of Chemistry, University of Canterbury, Christchurch, NEW ZEALAND

20. Gas phase reactions of group 15 EI_2^+ ions (E = P, As, Sb, and Bi) with n-butyl benzene: periodic changes in the reactivity of group 15 elements
Heinrich L. Sievers, Hans-Friedrich Grützmacher, and Dirk Kirchhoff
University of Bielefeld, Department of Chemistry, P.O.B. 100131, D-33501 Bielefeld Germany

21. Even/Odd Alternation in Styrene Cluster Ions and Intracluster Proton Transfer Reactions
Y. B. Pithawalla, Zhongde Yu, J. Gao, and M. Samy El-Shall
Department of Chemistry, Virginia Commonwealth University, Richmond, VA 23284-2006

22. Distonic Carbene Negative Ions
Jun Hu, Brian T. Hill, Robert R. Squires
Purdue University, Department of Chemistry, West Lafayette, IN 47907-1393

23. Influence of location of ionizing proton(s) on fragmentation of peptides.

Vicki H. Wysocki and Hari Nair,

RN#231, Old Chemistry bldg, Department of Chemistry, University of Arizona,
Tucson, AZ 85721

24. Molecular Dynamics Simulation of Gas Phase Ion Solvation

Orlando M. Cabarcos and James M. Lisy

School of Chemical Sciences, 600 S. Mathews Ave., Box 31-6, Urbana, IL 61801

25. Ion Photodissociation Kinetic Energy Release in an Octopole Ion Guide

Skip Williams, Rainer Dressler, Dale Levandier, and Edmond Murad

Phillips Laboratory/GPOS, 29 Randolph Rd., Hanscom AFB, MA 01731-3010

Tuesday Posters

1. Collision Induced Dissociation within Multiply Charged Ammonia Clusters

Eric Rexer, Robert L. DeLeon, and James F. Garvey

Department of Chemistry, Natural Sciences & Mathematics Complex

State University of New York, University at Buffalo, Buffalo, NY 14260-3000

2. Photoinitiating the S_N2 Reaction, NO₂⁻ + CH₃X → X⁻ + CH₃NO₂ (X = Cl, Br, and I): Using Dipole-Bound Excited States as Doorways to the Electronic Excited States of S_N2 Reactions

Caroline E.H. Dessent and Mark A. Johnson

Department of Chemistry, Yale University, New Haven, Conn.

3. Photoelectron Spectroscopy of Small Cluster Anions; Dipole Bound, Ground State Systems, and their Evolution toward Solvated Electron Species

Helen L. de Clercq, J.H. Hendricks, S.a. Lypustina, and K.H. Bowen

Department of Chemistry, The Johns Hopkins University, Baltimore, MD 21218

4. Rate Coefficients for the Endothermic Reactions: C(²P) + H₂ (D₂) → CH⁺ (CD⁺) + H (D) as Functions of Temperature from 400 - 1300 K

Peter M. Hierl^a, Robert A. Morris, and A.A. Viggiano

Phillips Laboratory, Geophysics Directorate, Ionosphere Effects Division (GPID); 29 Randolph R. Hanscom AFB, MA 01731-3010

a) Permanent Address: Department of Chemistry, University of Kansas, Lawrence, KS 66045-0046

5. Symmetry Induced Kinetic Isotope Effects in the formation of CO₂⁺ + Ar

Gregory I. Gellene and R. K. Yoo

Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409-1061

6. Delayed ejection of phenylethanethiol from a self-assembled monolayer upon ion beam bombardment.

Donald E. Riederer and Nicholas Winograd

Department of Chemistry, 123 Chemistry Building, University of Missouri, Columbia, MO 65211

7. Low energy collision-induced dissociation and photodissociation studies of the (N₂O,H₂O)⁺ cluster ion

Rainer A. Dressler, Dale J. Levandier, Peter B. Armentrout, Michael J. Bastian, Edmond Murad, and Felician Muntean

PL/GPOS, Hanscom AFB, MA 01731-3010; and Department of Chemistry, University of Utah, Salt Lake City, UT 84112

8. Cluster formation and its role in the process of Matrix Assisted Laser Desorption

J. Grottemeyer and A. Meffert

Am Technologiepark 1, 03099 Kolkwitz, Germany

9. Olefin Oxidation by Transition-Metal Dioxides: [2+2] versus [3+2] Route

Detlef Schröder, Jeremy N. Harvey, and Helmut Schwarz

Department of Chemistry, Technical University of Berlin, Strasse des 17 Juni 135 D-10623 Berlin, Germany

10. Gas phase ion-molecule reactions in the identification of chemical warfare related agents in an ion trap mass spectrometer

Sunia Afzaal

Bruker Analytical Instruments, Inc., 19 Fortune Dr. Billerica, MA

11. The Structures and Proton Affinities of Mono-Substituted Phenyl Anions, C₆H₄X⁻ (X = F, Cl, Br, CH₃, C₂H₅, NH₂, OCH₃, CN, CHO, NO₂ and CF₃): A Theoretical Study

Ming Wah Wong

Department of Chemistry, The University of Queensland, Brisbane, QLD 4072, Australia

12. Energetics of Ethylsilane Ion Dissociations Studied by TPEPICO

Jeffrey W. Keister, Paivi Tomperi, Ryan Biddell and Tomas Baer

Chemistry Department, University of North Carolina, Chapel Hill, NC 27599-3290

13. The Gas-Phase Neutral Chemistry of C₂H₂N Radicals: Implications for the Ion Surface.

Paul M. Mayer, Mark S. Taylor, Chris J. Parkinson, and Leo Radom

Research School of Chemistry, Australian National University, Canberra, ACT 0200 Australia

14. Structural Dichotomy in the Electronic States of the CrO₂²⁺ Di-cation

Ilona Kretzschmar, Andreas Fiedler, Detlef Schröder, and Helmut Schwarz

Technische Universität Berlin, D-10623 Berlin, Germany

15. Absolute cross sections of charge transfer reactions of sodium with N₂⁺, NO⁺ and O₂⁺: a guided-ion beam study.

Dale J. Levandier, Rainer A. Dressler, Skip Williams, and Edmond Murad

PL/GPOS, 29 Randolph Road, Hanscom AFB, MA 01731-3010

16. Intramolecular proton bridges in peptides: Effects on fragmentation.

Richard W. Vachet, T. Joon Lee, and Michael R. Asam, and Gary Glish

Chemistry Department, University of North Carolina, Chapel Hill, NC 27599-3290

17. Infrared Photodissociation of Proton Bound Dimers in a FTICR Spectrometer: A study of the interaction of radiation and ions under collision free conditions.

D. Scott Tonner and T.B. McMahon

Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1 CANADA

18. Evaporation Dynamics of $\text{Na}^+(\text{Methanol})_{2-8}$

Corey J. Weinheimer and James M. Lisy

School of Chemical Sciences, 600 S. Mathews Ave., Box 48-6, Urbana, IL 61801

19. Chemical Characterization of Radical Anions

Joseph J. Grabowski, Daniel Owusu, and Jiang Zhao

Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260

20. Low Energy Guided Ion Scattering for Isomer Analysis.

Zhi Li and Scott Anderson

Department of Chemistry, University of Utah, Salt Lake City, Utah, 84112

21. Electron-Molecular Ion Interactions at Low Energy

Lars Andersen

Institute of Physics and Astronomy, Aarhus University, DK8000 Aarhus C, Denmark
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22. Bond Strengths in Polyhalide Ions

Lee Sunderlin, Cynthia Pommerening, Katrina Nizzi, Khanh Do, and Timothy Klein

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Wednesday Posters

1. Collision Induced Dissociation of Mass Selected Ethylene Cluster Ions ($n=2-7$)

Michael Y. M. Lyktev, T. Rycroft, and James F. Garvey

Department of Chemistry, NSM Complex, State University of New York at Buffalo, Buffalo, NY 14260

2. Experimental and Theoretical Investigation of $\text{FSi}(\text{OCH}_3)_2(\text{OCH}_2)^-$: A Gas Phase Fluoride-Silaoxirane Adduct

Nelson H. Morgan,‡ Andre B. Argenton, Maria L. P. da Silva and José M. Riveros

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3. Sequential Dehydrogenation of Hydrocarbons by W^+ in the Gas Phase

G. Ohanessian, P. Mourgues, A. Ferhati, T. B. McMahon

Laboratoire des Mécanismes Réactionnels, Ecole Polytechnique, URA CNRS 1307, 91128 Palaiseau Cedex, FRANCE

4. Absolute Total Cross Section Study of the Dissociation Reaction of CH_3OH^+ by Collisional Activation

Yu-Ju Chen, P.T. Fenn, and C.Y. Ng

Department of Chemistry, Iowa State University, Ames, IA 50011

5. The Fragmentation of Long-lived Protonated Alkylcycloheptatrienes

Dietmar Kuck and Michael Mormann

Department of Chemistry, University of Bielefeld, Germany

6. The Neutral Fragments Formed by Decomposing Biomolecular and Cluster Ions

Chrys Wesdemiotis, Blas A. Cerdá, Michael J. Polce, and Da Ren

Department of Chemistry, The University of Akron, Akron, OH 44325-3601

7. Energy dependence of the proton transfer system $\text{H}_3\text{O}^+ + \text{CH}_2\text{O} \rightarrow \text{CH}_2\text{OH}^+ + \text{H}_2\text{O}$

W. Lindinger, A. Hansel, W. Singer, A. Wisthaler, and M. Schwarzm

Institut für Ionenphysik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, AUSTRIA

8. Energy dependence of the isomerization of HCN^+ to HNC^+ via ion molecule reactions

W. Lindinger, A. Hansel, M. Glantschnig, Ch. Scheiring, and E.E. Ferguson

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9. Comparative ab initio and hybrid DFT studies relevant to an experimental investigation of neutral and cationic $[\text{Si},\text{P},\text{H}_2]$ isomers

Jan Hrušák, Detlef Schröder¹, Helmut Schwarz¹, and Suehiro Iwata²

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2) Institute for Molecular Sciences, Myodaiji, 444 Okazaki, Japan

10. NeNuPo spectroscopy and femtosecond dynamics of neutral silver trimer

Doo Wan Boo, Yasushi Ozaki, and W. Carl Lineberger

JILA, University of Colorado, Campus Box 440, Boulder, CO 80309

11. Nitrogen Fixation by Transition Metal Oxo Complexes

Martin Beyer, Christian Berg, Gerhard Albert, Uwe Achatz, Stefan Joos, Gereon Niedner-Schatteburg, and Vladimir E. Bondybey

Institut für Physikalische und Theoretische Chemie, TU München, Lichtenbergstrasse 4, 85356 Garching, Germany

12. Differential NR/CR Spectra to Examine the Neutrals' Reactivity

Detlef Schröder, Christoph A. Schalley, and Helmut Schwarz

Department of Chemistry, Technical Univ. of Berlin, Strasse des 17 Juni 135, D-10623 Berlin, Germany

13. Collision Induced-dissociation dynamics of the enolic acetone cation: Evidence for non-ergodic behavior

Runzhi Zhao, Ronald Tosh, Anil Shukla, and Jean Futrell

Department of Chemistry, University of Delaware, Newark, DE 19716

14. Vibrational-rotational state selectivity in chemical reactions: Gas phase proton transfer reactions



Hiroto Tachikawa

Graduate School of Engineering, Hokkaido University, Sapporo 060, Japan

15. Application of REMPI to High pressure Mass Spectrometry: Polymerization of Propene Initiated by Charge Transfer from Benzene Radical Cation

M. Samy El-Shall, Y. B. Pithawalla, Junling Gao and M. Meot-Ner

Department of Chemistry, Virginia Commonwealth University, Richmond, VA 23284-2006

16. Fundamentals of CID with FT-ICR mass spectrometry: approaching time and collision-energy resolved mass spectrometry

Heinrich L. Sievers, and Hans-Friedrich Grützmacher

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17. Thermochemistry of Reactive Intermediates from Collision-Induced Dissociation Experiments: The Heat of Formation of Cyclopropylidene and the Electron Affinity of Cyclopropyl Radical

Randal A. Seburg and Robert R. Squires

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18. Theoretical Modeling of Bimolecular Ion-Molecule Dynamics:

Ni⁺ Reactions with C₃H₈ and n-C₄H₁₀

Sung Soo Yi, James C. Weisshaar, M. R. A. Blomberg, and P. E. M. Siegbahn

Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin
and Department of Physics, University of Stockholm, Stockholm, Sweden

19. Bimolecular Ion-Molecule Dynamics in Real Time: Co⁺ and Ni⁺ Reactions with C₃H₈ and n-C₄H₁₀

Sung Soo Yi, R. J. Noll, and James C. Weisshaar

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20. Ion-surface Reactions on Langmuir-Blodgett Films

Vicki H. Wysocki and Chungang Gu

Department of Chemistry, University of Arizona, Tucson, AZ 85721-0041

21. Two-Component Dissociation Dynamics of Energy Selected Methyl Formate Ions

Oleg A. Mazyar and Tomas Baer

Chemistry Department, University of North Carolina, Chapel Hill, NC 27599-3290

22. Low energy reactive and dissociative collisions of polyatomic ions and dimer ions with a solid surface

Grill and T. D. Märk

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